

10/552,595D part 04/24/2009 Yong Chu

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SESSION RESUMED IN FILE 'REGISTRY' AT 10:32:38 ON 24 APR 2009  
FILE 'REGISTRY' ENTERED AT 10:32:38 ON 24 APR 2009  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	210.84	211.06

=> d his

(FILE 'HOME' ENTERED AT 09:51:22 ON 24 APR 2009)

FILE 'REGISTRY' ENTERED AT 09:51:38 ON 24 APR 2009

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 STRUCTURE UPLOADED

L4 12498 S L1 FULL

SAVE L4 YC105525957A

L5 STRUCTURE UPLOADED

L6 STRUCTURE UPLOADED

L7 STRUCTURE UPLOADED

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	211.32	211.54

FILE 'REGISTRY' ENTERED AT 10:33:00 ON 24 APR 2009  
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STRUCTURE FILE UPDATES: 22 APR 2009 HIGHEST RN 1138219-76-7  
DICTIONARY FILE UPDATES: 22 APR 2009 HIGHEST RN 1138219-76-7

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when  
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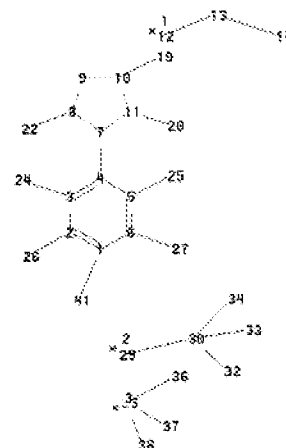
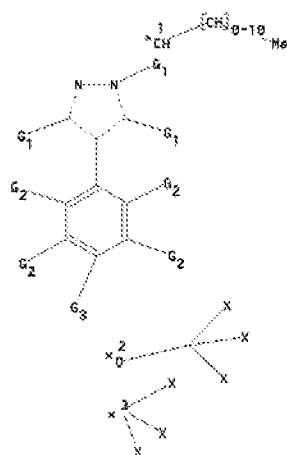
REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
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=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10552595\L14\_04242009.str



chain nodes :

12 13 14 19 20 22 24 25 26 27 29 30 32 33 34 35 36 37 38 41

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-41 2-26 3-24 4-7 5-25 6-27 8-22 10-19 11-20 12-13 13-14 29-30 30-32  
30-33 30-34 35-36 35-37 35-38

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11

exact/norm bonds :

1-41 2-26 3-24 5-25 6-27 7-8 7-11 8-9 8-22 9-10 10-11 10-19 11-20 29-30

exact bonds :

4-7 12-13 13-14 30-32 30-33 30-34 35-36 35-37 35-38

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:CH3,H, [\*1]

G2:H,CH3

G3:G1,OH,SH,CN,NH2,NO2,X, [\*2], [\*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:CLASS 13:CLASS 14:CLASS 19:CLASS 20:CLASS 22:CLASS 24:CLASS  
25:CLASS 26:CLASS  
27:CLASS 29:CLASS 30:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS  
37:CLASS 38:CLASS  
41:CLASS

L8            STRUCTURE UPLOADED

=> d

L8 HAS NO ANSWERS

L8            STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l8 sam sss sub=l4

SAMPLE SUBSET SEARCH INITIATED 10:33:38 FILE 'REGISTRY'

SAMPLE SUBSET SCREEN SEARCH COMPLETED -        639 TO ITERATE

100.0% PROCESSED        639 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):

ONLINE    \*\*COMPLETE\*\*

PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):

11264 TO    14296

PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):

3 TO        163

L9            3 SEA SUB=L4 SSS SAM L8

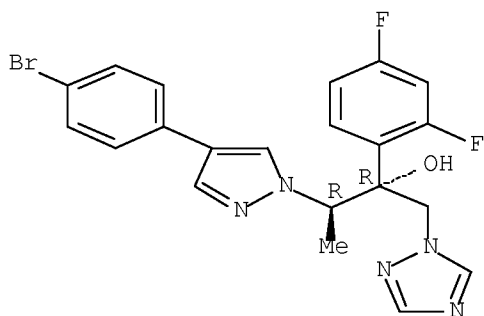
=> d scan

L9    3 ANSWERS    REGISTRY    COPYRIGHT 2009 ACS on STN

IN    1H-1,2,4-Triazole-1-ethanol, .alpha.-[(1R)-1-[4-(4-bromophenyl)-1H-pyrazol-1-yl]ethyl]-.alpha.-(2,4-difluorophenyl)-, (.alpha.R)-

MF    C21 H18 Br F2 N5 O

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l8 full sss sub=l4

FULL SUBSET SEARCH INITIATED 10:34:21 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED -        12498 TO ITERATE

100.0% PROCESSED 12498 ITERATIONS  
SEARCH TIME: 00.00.01

59 ANSWERS

L10 59 SEA SUB=L4 SSS FUL L8

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

44.96

256.50

FILE 'CAPLUS' ENTERED AT 10:34:26 ON 24 APR 2009

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FILE COVERS 1907 - 24 Apr 2009 VOL 150 ISS 18

FILE LAST UPDATED: 23 Apr 2009 (20090423/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l10

L11 41 L10

=> save l11

ENTER NAME OR (END):yc10552595A/A

ANSWER SET L11 HAS BEEN SAVED AS 'YC10552595A/A'

=> d ibib abb hitstr 30-41

'ABB' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB

ALL ----- BIB, AB, IND, RE

APPS ----- AI, PRAI

BIB ----- AN, plus Bibliographic Data and PI table (default)

CAN ----- List of CA abstract numbers without answer numbers

CBIB ----- AN, plus Compressed Bibliographic Data

CLASS ----- IPC, NCL, ECLA, FTERM

DALL ----- ALL, delimited (end of each field identified)

DMAX ----- MAX, delimited for post-processing

FAM ----- AN, PI and PRAI in table, plus Patent Family data  
 FBIB ----- AN, BIB, plus Patent FAM  
 IND ----- Indexing data  
 IPC ----- International Patent Classifications  
 MAX ----- ALL, plus Patent FAM, RE  
 PATS ----- PI, SO  
 SAM ----- CC, SX, TI, ST, IT  
 SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;  
                   SCAN must be entered on the same line as the DISPLAY,  
                   e.g., D SCAN or DISPLAY SCAN)  
 STD ----- BIB, CLASS  
  
 IABS ----- ABS, indented with text labels  
 IALL ----- ALL, indented with text labels  
 IBIB ----- BIB, indented with text labels  
 IMAX ----- MAX, indented with text labels  
 ISTD ----- STD, indented with text labels  
  
 OBIB ----- AN, plus Bibliographic Data (original)  
 OIBIB ----- OBIB, indented with text labels  
  
 SBIB ----- BIB, no citations  
 SIBIB ----- IBIB, no citations  
  
 HIT ----- Fields containing hit terms  
 HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)  
                   containing hit terms  
 HITRN ----- HIT RN and its text modification  
 HITSTR ----- HIT RN, its text modification, its CA index name, and  
                   its structure diagram  
 HITSEQ ----- HIT RN, its text modification, its CA index name, its  
                   structure diagram, plus NTE and SEQ fields  
 FHITSTR ----- First HIT RN, its text modification, its CA index name, and  
                   its structure diagram  
 FHITSEQ ----- First HIT RN, its text modification, its CA index name, its  
                   structure diagram, plus NTE and SEQ fields  
 KWIC ----- Hit term plus 20 words on either side  
 OCC ----- Number of occurrence of hit term and field in which it occurs

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All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.  
 ENTER DISPLAY FORMAT (BIB):end

=> d ibib abs hitstr 30-41

L11 ANSWER 30 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1981:568095 CAPLUS Full-text  
 DOCUMENT NUMBER: 95:168095  
 ORIGINAL REFERENCE NO.: 95:28085a,28088a  
 TITLE: Free-radical reactions of diazonium salts with  
           .alpha.,.beta.-unsaturated carbonyl compounds. A new  
           synthesis of 1,4-diarylpyrazole derivatives

AUTHOR(S): Citterio, Attilio; Ramperti, Massimo; Vismara, Elena  
CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, 20133, Italy  
SOURCE: Journal of Heterocyclic Chemistry (1981), 18(4), 763-6  
CODEN: JHTCAD; ISSN: 0022-152X

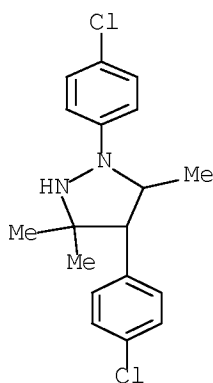
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 95:168095

AB Free-radical decompn. of benzene diazonium salts catalyzed by titanous or titanous and ferrous salts in th presence of .beta.-substituted .alpha.,.beta.-unsatd. carbonyl compds., e.g., 4-methyl-3-pentene-2-one, Me 2-butenolate, leads to 1,4-diarylpyrazole derivs. The reaction occurs via an intermediate azo compds., which can be reduced by the metal salt or can be isolated and hydrogenated to pyrazole derivs.

IT 79481-66-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 79481-66-6 CAPLUS

CN Pyrazolidine, 1,4-bis(4-chlorophenyl)-3,3,5-trimethyl- (CA INDEX NAME)



L11 ANSWER 31 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:179094 CAPLUS Full-text

DOCUMENT NUMBER: 84:179094

ORIGINAL REFERENCE NO.: 84:29023a,29026a

TITLE: Anisotropy effects of conjugated cyclic systems, I.  
NMR spectra of mesityl- and (9-anthryl)-substituted  
aromatic compounds

AUTHOR(S): Bock, Bodo; Kuhr, Manfred; Musso, Hans  
CORPORATE SOURCE: Inst. Org. Chem., Univ. Karlsruhe, Karlsruhe, Fed.  
Rep. Ger.

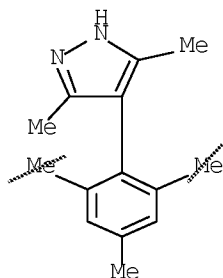
SOURCE: Chemische Berichte (1976), 109(3), 1184-94  
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal  
LANGUAGE: German

AB Magnetic anisotropies in mesityl and 9-anthryl derivs of benzene, mesitylene, anthracene, pyrimidine, pyrazole, and isoxazole were measured via 1H-NMR chem. shift data. The chem. shift differences of the 1-H and 4-H signals of 9-anthryl substituents are a measure of the magnetic anisotropy of arom. systems.

IT 59146-22-4  
RL: PRP (Properties)  
(NMR of)

RN 59146-22-4 CAPLUS  
CN 1H-Pyrazole, 3,5-dimethyl-4-(2,4,6-trimethylphenyl)- (CA INDEX NAME)



L11 ANSWER 32 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1975:175242 CAPLUS Full-text  
DOCUMENT NUMBER: 82:175242  
ORIGINAL REFERENCE NO.: 82:27995a,27998a  
TITLE: Compositions of  
1,2-dialkyl-3(and/or4)-aryl-3-pyrazolines and salts  
and method of lowering blood sugar levels with them  
INVENTOR(S): Jacquier, Robert  
PATENT ASSIGNEE(S): Schering A.-G., Fr.  
SOURCE: U.S., 9 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3818095	A	19740618	US 1972-243427	19720412
PRIORITY APPLN. INFO.:			US 1972-243427	19720412

GI For diagram(s), see printed CA Issue.

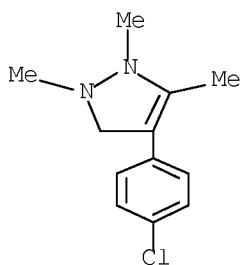
AB 2-Pyrazolinium perchlorates (I) were prepd. and used in pharmaceutical compns. as hypoglycemics. Thus propiophenone [93-55-0], MeNHNHMe.2HCl [306-37-6], and HCHO [50-00-0] in EtOH with HCl were heated at reflux for 5 hr and worked up to give 1,2,4-trimethyl-3-phenyl-3-pyrazoline (II) [18508-29-7]. II (and other pyrazolines) were treated with HClO<sub>4</sub> to give the perchlorate salts with a shift of the double bond to position 2. A tablet formulation contained, e.g., 50 mg/tablet 1,2,4-trimethyl-3-phenyl-2-pyrazolinium perchlorate [18075-75-7].

IT 51771-94-9P 51772-13-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 51771-94-9 CAPLUS

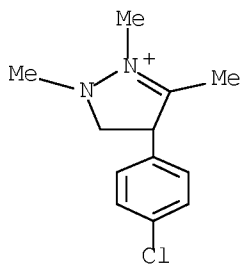
CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl- (CA INDEX NAME)



RN 51772-13-5 CAPLUS  
 CN 1H-Pyrazolium, 4-(4-chlorophenyl)-4,5-dihydro-1,2,3-trimethyl-,  
 perchlorate (1:1) (CA INDEX NAME)

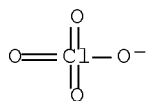
CM 1

CRN 51772-12-4  
 CMF C12 H16 Cl N2



CM 2

CRN 14797-73-0  
 CMF Cl O4



L11 ANSWER 33 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1974:496468 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 81:96468  
 ORIGINAL REFERENCE NO.: 81:15239a,15242a  
 TITLE: Compositions of 1,2-alkyl arylpyrazolium quaternary  
 salts and lowering blood sugar levels with same



INVENTOR(S): Sherlock, Margaret  
 PATENT ASSIGNEE(S): Schering Corp.  
 SOURCE: U.S., 10 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3818096	A	19740618	US 1972-243429	19720412

PRIORITY APPLN. INFO.: US 1972-243429 19720412

AB Compsn. for lowering blood sugar levels in warm blooded animals suffering from hyperglycemia consist of a pharmaceutical carrier and I. Thus, to Ph3CCl in MeCN was added 1,2-dimethyl-3-phenyl-3-pyrazoline in MeCN to give after workup 1,2-dimethyl-3-phenylpyrazolium chloride (II), m.p. 190-2.degree. (decompn.). Tablets are prepd. contg. II 100.00, confectioner's sugar (food grade) 123.00, polyvinylpyrrolidone (PVP) 10.00, corn starch (food grade, dried) 13.00, SiO2 2.00, and Mg sterate (U.S.P.) 2.00 mg/tablet. A damp mass consisting of II, the sugar, and PVP is prepd., dried, and reduced to granules. The starch, SiO2, and Mg stearate are added and mixed in. The compn. is then compressed into tablets.

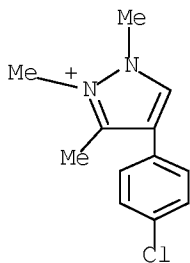
IT 54156-57-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (antihyperglycemic, prepn. of)

RN 54156-57-9 CAPLUS

CN 1H-Pyrazolium, 4-(4-chlorophenyl)-1,2,3-trimethyl-, (2E)-2-butenedioate  
 (1:1) (9CI) (CA INDEX NAME)

CM 1

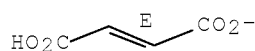
CRN 54156-56-8  
 CMF C12 H14 Cl N2



CM 2

CRN 18610-40-7  
 CMF C4 H3 O4

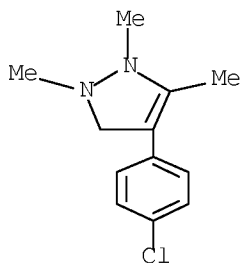
Double bond geometry as shown.



L11 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1974:120928 CAPLUS Full-text  
 DOCUMENT NUMBER: 80:120928  
 ORIGINAL REFERENCE NO.: 80:19467a,19470a  
 TITLE: Antiglycemic 3-pyrazolines  
 PATENT ASSIGNEE(S): Laboratoire Cetrane  
 SOURCE: Fr. Demande, 39 pp.  
 CODEN: FRXXBL  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2179559	A1	19731123	FR 1972-12761	19720412
FR 2179559	B1	19750425		

PRIORITY APPLN. INFO.: FR 1972-12761 19720412  
 GI For diagram(s), see printed CA Issue.  
 AB Pyrazoles I, II, and III (R = Me, Ph, substituted phenyl; R1 = H, Me, Et, Ph, p-ClC6H4; R2 = H, Me, Ph; X = ClO4, iodide, fumarate) (56 compds.), were prepd. Condensation of RCOCHR1CH2R2 or RCOCHR1COR2 with MeNHNHMe.2HCl and paraformaldehyde gave I or II, resp. LiAlH4 redn. of II gave pyrazolinium III.  
 IT 51771-94-9P 51772-13-5P 51772-18-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 51771-94-9 CAPLUS  
 CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl- (CA INDEX NAME)

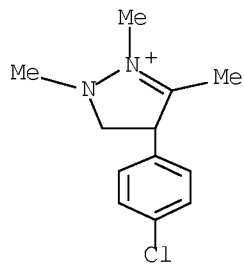


RN 51772-13-5 CAPLUS  
 CN 1H-Pyrazolium, 4-(4-chlorophenyl)-4,5-dihydro-1,2,3-trimethyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 51772-12-4

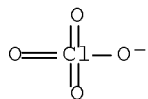
CMF C12 H16 Cl N2



CM 2

CRN 14797-73-0

CMF Cl O4



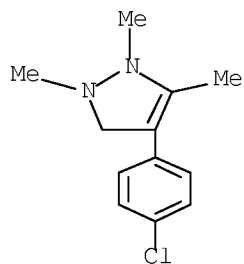
RN 51772-18-0 CAPLUS

CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl-,  
(2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 51771-94-9

CMF C12 H15 Cl N2

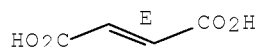


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



L11 ANSWER 35 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1974:108434 CAPLUS Full-text

DOCUMENT NUMBER: 80:108434

ORIGINAL REFERENCE NO.: 80:17443a,17446a

TITLE: Reactivity of 4-diazo-3,5-dimethylpyrazole. IV.  
Catalytic action of hydroquinone in the  
Gomberg-Bachmann reaction

AUTHOR(S): Fukata, Gouki; Kawazoe, Yuichi; Taguchi, Tanezo

CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, Japan

SOURCE: Yakugaku Zasshi (1974), 94(1), 36-43

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

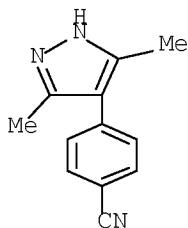
AB Refluxing 4-diazo-3,5-dimethylpyrazole (I) in benzene for a long time afforded 4-phenyl-3,5-dimethylpyrazole, 1H,4H-3-methylpyrazolo[4,3-c]-pyrazole, 3,5-dimethylpyrazole, and biphenyl in 36, 15, 12, and 7% yields, resp. Replacement of benzene with nitrobenzene in this reaction gave o-, m-, and p-isomers of 4-(nitrophenyl)-3,5-dimethylpyrazole in a ratio of 10:2.8:3.0. In these reactions, addn. of hydroquinone (catalytic quantity, 5% by wt. of I) was very effective in increasing the yield of 4-aryl-3,5-dimethylpyrazole and reduction of reaction time. The intermediate in these reactions was a diazonium salt which was formed by the addn. of one mole of hydroquinone to two moles of I.

IT 51463-73-1P

RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, by refluxing diazodimethylpyrazole in benzonitrile)

RN 51463-73-1 CAPLUS

CN Benzonitrile, 4-(3,5-dimethyl-1H-pyrazol-4-yl)- (CA INDEX NAME)

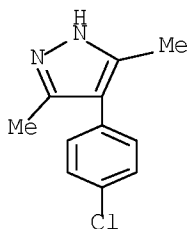


IT 51463-76-4P

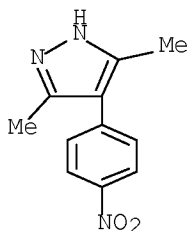
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, by refluxing diazodimethylpyrazole in chlorobenzene)

RN 51463-76-4 CAPLUS

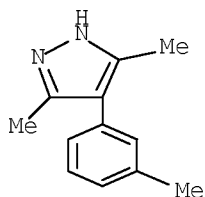
CN 1H-Pyrazole, 4-(4-chlorophenyl)-3,5-dimethyl- (CA INDEX NAME)



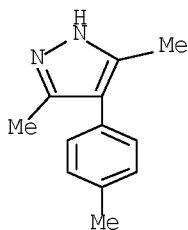
IT 42418-61-1P  
 RL: FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation of, by refluxing diazodimethylpyrazole in nitrobenzene)  
 RN 42418-61-1 CAPLUS  
 CN 1H-Pyrazole, 3,5-dimethyl-4-(4-nitrophenyl)- (CA INDEX NAME)



IT 51463-81-1P 51463-82-2P  
 RL: FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation of, by refluxing diazodimethylpyrazole in toluene)  
 RN 51463-81-1 CAPLUS  
 CN 1H-Pyrazole, 3,5-dimethyl-4-(3-methylphenyl)- (CA INDEX NAME)

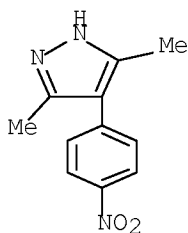


RN 51463-82-2 CAPLUS  
 CN 1H-Pyrazole, 3,5-dimethyl-4-(4-methylphenyl)- (CA INDEX NAME)



~~\*\*102b\*\*~~ Cited ref

L11 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1973:452480 CAPLUS Full-text  
 DOCUMENT NUMBER: 79:52480  
 ORIGINAL REFERENCE NO.: 79:8467a,8470a  
 TITLE: Reactivity of 4-diazo-3,5-dimethylpyrazole  
 AUTHOR(S): Fukata, Gouki; Kawazoe, Yuichi; Taguchi, Tanezo  
 CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, Japan  
 SOURCE: Tetrahedron Letters (1973), (15), 1199-200  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB The title compd. (I) was heated in Me3COH-AcOH, Me3COH, and EtOH to give 70% II, 45% III, and 85% MeCHO resp. Heating I in C6H6 gave 15% II, 12% 3,5-dimethylpyrazole, 7% biphenyl, and 36% IV. Hydroquinone and benzoquinone catalyzed the reaction giving IV (68%). III was also obtained by coupling I with II in Me3COH. Heating I in PhNO2 gave 4-nitrophenyl-3,5-dimethylpyrazole with a ratio of o:m:p-isomers = 10:3:3.  
 IT 42418-61-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 42418-61-1 CAPLUS  
 CN 1H-Pyrazole, 3,5-dimethyl-4-(4-nitrophenyl)- (CA INDEX NAME)



L11 ANSWER 37 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1972:539882 CAPLUS Full-text  
 DOCUMENT NUMBER: 77:139882  
 ORIGINAL REFERENCE NO.: 77:23001a,23004a  
 TITLE: Pyrazoles. IX. Nitration of  
 1-methyl-4-phenylpyrazole  
 AUTHOR(S): Cohen-Fernandes, Pauline; Habraken, Clarisse L.  
 CORPORATE SOURCE: Gorlaeus Lab., Univ. Leiden, Leiden, Neth.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1972),  
 91(9-10), 1185-92  
 CODEN: RTCPA3; ISSN: 0165-0513

DOCUMENT TYPE: Journal

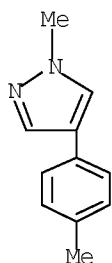
LANGUAGE: English

AB The phenyl and the pyrazole ring were both substituted on nitration with  
 acetyl nitrate and a predominant ortho substitution in the phenyl ring was  
 obsd. The pyrazole ring was susceptible to nitration at positions other than  
 the, hitherto favored, 4-position.

IT 37921-11-2P 37921-15-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

RN 37921-11-2 CAPLUS

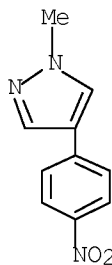
CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



~~\*\*102b\*\*~~

RN 37921-15-6 CAPLUS

CN 1H-Pyrazole, 1-methyl-4-(4-nitrophenyl)- (CA INDEX NAME)



L11 ANSWER 38 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1963:46687 CAPLUS Full-text

DOCUMENT NUMBER: 58:46687

ORIGINAL REFERENCE NO.: 58:7921a-c

TITLE: Derivatives of 3-substituted pyrazolones and  
 3-substituted pyrazolines

AUTHOR(S): Kurihara, Tozaburo; Takeda, Hideo; Iino, Naoko

CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai

SOURCE: Tohoku Yakka Daigaku Kiyo (1961), 8, 103-9  
 CODEN: TYDKAG; ISSN: 0372-347X

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB 1-Phenyl-3-chloro-4-pyrazoolone (1.9 g.) was warmed with 0.9 g. Me<sub>2</sub>NH in MeOH in an autoclave 2 hrs. to give 1-phenyl-3-dimethylamino-5-pyrazolone, m. 132.degree. (EtOH). Similarly prepd. were the following I (R, R<sub>1</sub>, R<sub>2</sub>, and m.p. given): H, H, NEt<sub>2</sub>, 131.degree.; H, H, (iso-Bu)<sub>2</sub>N, 108.degree.; H, Br, (iso-Bu)<sub>2</sub>N, 138-40.degree.; H, Cl, (iso-Bu)<sub>2</sub>N, 126.degree.; H, H, piperidyl, 139.degree.; H, H, morpholyl, 134.degree.; Bu, H, morpholyl, 225.degree.; H, Br, morpholyl, 165.degree.; H, Cl, morpholyl, 143.degree.; H, Me, morpholyl, 168-170.degree.; H, OMe, morpholyl, 127-30.degree.; H, H, Et<sub>2</sub>NCH<sub>2</sub>NH, 202.degree.; H, H, Et<sub>2</sub>NCH<sub>2</sub>CONH, 158.degree.; H, H, morpholylacetamido.

IT 94628-08-7  
(Derived from data in the 7th Collective Formula Index (1962-1966))

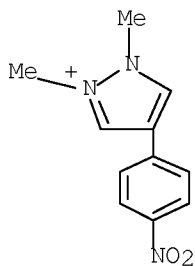
RN 94628-08-7 CAPLUS

CN 1H-Pyrazolium, 1,2-dimethyl-4-(4-nitrophenyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 94628-07-6

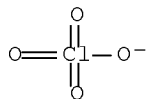
CMF C11 H12 N3 O2



CM 2

CRN 14797-73-0

CMF Cl O4



L11 ANSWER 39 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1963:46686 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 58:46686

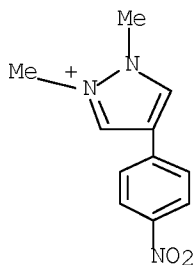
ORIGINAL REFERENCE NO.: 58:7920h, 7921a

TITLE: The 1,2-dithiolium cation. A new pseudoaromatic system. III. Conversion of dithiolium salts to quaternary pyrazolium salts and dithiolethiones

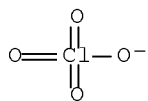
AUTHOR(S): Klingsberg, Erwin



CORPORATE SOURCE: Am. Cyanamid Co., Bound Brook, NJ  
 SOURCE: Journal of Organic Chemistry (1963), 28, 529-30  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 58:46686  
 GI For diagram(s), see printed CA Issue.  
 AB cf. CA 57, 16791e. 4-Phenyl-(I) and 4-p-nitrophenyl-1,2-dithiolium salts react with N,N'-disubstituted hydrazines to give N,N-disubstituted pyrazolium salts, e.g., II, and with sulfur to give 1,2-dithiole-3-thiones, e.g. III.  
 IT 94628-08-7P, 1,2-Dimethyl-4-(p-nitrophenyl)pyrazolium perchlorate  
 RL: PREP (Preparation)  
 (prepn. of)  
 RN 94628-08-7 CAPLUS  
 CN 1H-Pyrazolium, 1,2-dimethyl-4-(4-nitrophenyl)-, perchlorate (1:1) (CA INDEX NAME)  
 CM 1  
 CRN 94628-07-6  
 CMF C11 H12 N3 O2



CM 2  
 CRN 14797-73-0  
 CMF C1 O4



L11 ANSWER 40 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1958:55872 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 52:55872  
 ORIGINAL REFERENCE NO.: 52:10061i,10062a-c  
 TITLE: Synthesis of 2-substituted-acenaphtheno(4',5'-4,5)imidazole derivatives  
 AUTHOR(S): Saikachi, Haruo; Tsuge, Otohiko; Yoshimura, Kazuki

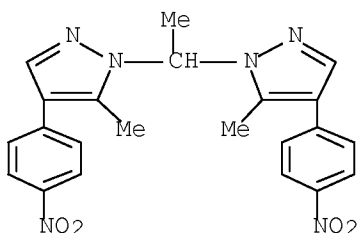
CORPORATE SOURCE: Kyushu Univ., Fukuoka  
SOURCE: Kogyo Kagaku Zasshi (1956), 59, 933-6  
CODEN: KGKZA7; ISSN: 0368-5462  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB cf. C.A. 52, 3779e. 4-Nitro-5-acylaminoacenaphthenes (I) (formyl, m. 226-7.degree.; Ac, 241.5-2.0.degree.; Bz, 228-9.degree.) were obtained from 5-amino-acenaphthene through the 5-acylaminoacenaphthene. Formyl and Ac derivs. of I were hydrolyzed by heating with EtOH-HCl 20 hrs. to give 4-nitro-5-aminoacenaphthene (II), m. 212-13.degree.. II was reduced with SnCl in HCl satd. EtOH to give 4,5-diaminoacenaphthene (III), m. 137.degree.. III (1 g.) with 3 cc. boiling 80% HCO<sub>2</sub>H gave 0.6 g. acenaphtheno(4',5'-4,5)imidazole, m. 221-2.degree.. III (1 g.) with 2 cc. Ac<sub>2</sub>O in C<sub>6</sub>H<sub>6</sub> on an H<sub>2</sub>O bath gave 0.6 g. 1-(N-acetyl)-2-methyl-acenaphtheno(4',5'-4,5)imidazole (IV), m. 263.degree.. Ac deriv. of I was reduced in Ac<sub>2</sub>O by Zn and converted to IV. The reduction of formyl deriv. of I in Ac<sub>2</sub>O with Zn by boiling gave 1-(N-carboxy) - 2 - methylacenaphtheno(4',5' - 4,5)imidazole, m. 279.degree., sol. in aq. NaOH. 4,5-Dibenzoyldiaminoacenaphthene, m. 282-3.degree., was obtained by boiling III with BzCl. III.HCl (1 g.) heated with 0.3 g. urea at 150-5.degree. 45 min. and extd. with aq. NaOH and then EtOAc gave acenaphtheno-(4',5'-4,5)-2-imidazolinone, m. above 340.degree.. Similarly, III.HCl with thiourea at 230.degree. or 450.degree. gave acenaphtheno-(4',5'-4,5)-2-thioimidazolinone, m. above 340.degree..

IT 102599-03-1P, Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)-  
nitrophenyl)-  
RL: PREP (Preparation)  
(prepn. of)

RN 102599-03-1 CAPLUS

CN Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)- (6CI) (CA INDEX NAME)



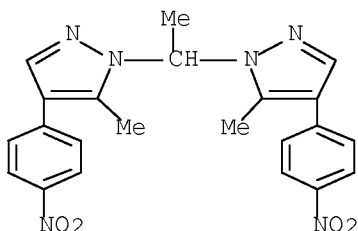
L11 ANSWER 41 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1958:55871 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 52:55871  
ORIGINAL REFERENCE NO.: 52:10061e-i  
TITLE: Products from the reaction of diazoethane with  
diazoketones  
AUTHOR(S): Yates, P.; Farnum, D. G.; Wiley, D. W.  
CORPORATE SOURCE: Harvard Univ.  
SOURCE: Chemistry & Industry (London, United Kingdom) (1958)  
69-70  
CODEN: CHINAG; ISSN: 0009-3068  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
GI For diagram(s), see printed CA Issue.

AB cf. C.A. 43, 4652g, 6992e. The structures  $\text{ArCOCR:NN:CHR'}$  ( $\text{R} = \text{R}' = \text{Me}$ ) (I) and ( $\text{R} = \text{H}$ ,  $\text{R}' = \text{Me}$ ) (II) ( $\text{Ar} = \text{p-O}_2\text{NC}_6\text{H}_4$  throughout) previously proposed (C.A. 43, 6992e) for the products of the reaction between  $\text{ARCOCRN}_2$  and  $\text{MeCHN}_2$  were confirmed. I, m. 99–100.degree.,  $\lambda$ . 265 m. $\mu$ . ( $\epsilon$ . 13,700),  $\lambda$ . 5.93, 6.06, 6.23  $\mu$ ., boiled 15 min. with 70% EtOH gave ( $\text{ArCOCMe:NNH}$ ) $_2$ CHMe (III), m. 159–60.degree.,  $\lambda$ . 268 and 315 m. $\mu$ . ( $\epsilon$ . 35,300 and 18,900),  $\lambda$ . 3.04, 6.03 (shoulder), 6.06, 6.24, 6.39  $\mu$ ., corresponding to the earlier compd.,  $\text{C}_{11}\text{H}_9\text{O}_2\text{N}_3$  (C.A. 43, 6992e). III with  $\text{Ac}_2\text{O}$  and  $\text{NaOAc}$  gave  $\text{ArCOCMe:NNHAc}$ , m. 165.5–6.5.degree.,  $\lambda$ . 245 and 278 m. $\mu$ . ( $\epsilon$ . 12,100 and 19,300),  $\lambda$ . 3.04, 5.81, 5.92, 5.99, 6.26  $\mu$ ., identical with the acetylated product of  $\text{ArCOCMe:NNH}_2$  (IV), m. 173–3.2.degree.,  $\lambda$ . 274 m. $\mu$ . ( $\epsilon$ . 14,200),  $\lambda$ . 2.92, 3.03, 3.31, 6.04, 6.16, 6.25, 6.36  $\mu$ ., obtained by  $\text{NH}_4\text{HS}$  reduction of  $\text{ArCOCMeN}_2$ . III with  $\text{BzH}$  gave  $\text{ArCOCMe:NN:CHPh}$ , m. 114.5–15.5.degree.,  $\lambda$ . 5.98, 6.18, 6.23, 6.40  $\mu$ ., also obtained from IV. I with IV 6 days in  $\text{CHCl}_3$  or refluxing in abs. EtOH gave III (63% yield by the 2nd method). I heated alone in abs. EtOH gave  $\text{ArCOCMe:NNHCHMeOEt}$ , m. 126–7.degree.,  $\lambda$ . 268 and 305 m. $\mu$ . ( $\epsilon$ . 17,750 and 11,000),  $\lambda$ . 3.03, 6.08, 6.24, 6.42  $\mu$ ., which was converted to III by treatment with aq. EtOH.  $\text{ArCOCHN}_2$  with  $\text{MeCHN}_2$  gave the 2 stereoisomers of II, A, m. 69–70.degree.,  $\lambda$ . 5.93, 6.09, 6.22  $\mu$ ., B, m. 121–2.degree. (decompn.),  $\lambda$ . 5.99, 6.09, 6.24, 6.29  $\mu$ .; A was converted to B by heating at its m.p. Further reaction of II with  $\text{MeCHN}_2$  gave  $\text{ArCOCMe:CHNHN:CHMe}$  (V), m. 136–6.5..degree.,  $\lambda$ . 298 m. $\mu$ . ( $\epsilon$ . 22,800),  $\lambda$ . 3.02, 6.08, 6.16, 6.31  $\mu$ ., corresponding to the earlier compd. (C.A. 43, 6992e),  $\text{C}_{14}\text{H}_{17}\text{O}_3\text{N}_3$ . Hydrolysis of V in cold 2N  $\text{HCl}$  gave 3-(p-nitrophenyl)-4-methylpyrazole (VI), m. 181.5–2.degree.,  $\lambda$ . 2.92, 3.13, 6.23  $\mu$ ., identified by nitration of the Ph analog, and  $[\text{ArC:Me.CH:N.N}]_2\text{CHMe}$ , m. 201.5–2.5.degree.,  $\lambda$ . 231 and 318 m. $\mu$ . ( $\epsilon$ . 22,500 and 21,800),  $\lambda$ . 6.24 and 6.44  $\mu$ .. Ultraviolet spectra were taken in  $\text{CH}_2\text{Cl}_2$ , infrared spectra in  $\text{CHCl}_3$ .

IT 102599-03-1P, Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)-  
nitrophenyl)-  
RL: PREP (Preparation)  
(prepn. of)

RN 102599-03-1 CAPLUS

CN Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)- (6CI) (CA INDEX  
NAME)



=>

=>

Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	71.18	327.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-9.84	-9.84

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